MPAS-JEDI 3D/4DEnVar

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NCAR | MESOSCALE & MICROSCALE METEOROLOGY

Overview

1. **Variational Cost Function**
2. Ensemble Error Covariance Matrix
3. Overview of 3DEnVar
4. Setting up a .yaml file for 3DEnVar
5. Overview of 4DEnVar
6. Setting up a .yaml file for 4DEnVar

The Problem

We want to find the **analysis state** (x) that minimizing a cost function with an optimal fit to the background and observations.

$$J(x) = \boxed{\frac{1}{2}(x - x_b)^T \mathbf{B}^{-1}(x - x_b)} + \boxed{\frac{1}{2}(h(x) - y)^T \mathbf{R}^{-1}(h(x) - y)}$$

Distance to background

Distance to observations

Incremental Cost Function in JEDI

Liu et al. (2022)

Full-form

$$J(x) = \frac{1}{2}(x - x_b)^T \boldsymbol{B}^{-1}(x - x_b) + \frac{1}{2}(h(x) - y)^T \boldsymbol{R}^{-1}(h(x) - y)$$

Incremental-form

$$J(\delta x) = \frac{1}{2}(\delta x - \delta x_g)^T \boldsymbol{B}^{-1}(\delta x - \delta x_g) + \frac{1}{2}(\boldsymbol{H}\delta x - d)^T \boldsymbol{R}^{-1}(\boldsymbol{H}\delta x - d)$$

$\boldsymbol{\delta x = x - x_g}$ $\delta x_g = x_b - x_g$ $\boldsymbol{d = y - h(x_g)}$

The minimization deals with increments to a known reference state

- Cost function minimizes δx=x− x_g instead of the full state (x)
- Start from $x_g = x_b$ and $\delta x_g = 0$
- **After minimization->** $x_a = x_g + \delta x$

Appropriately assign B and R is critical

We want to find the analysis state (x) that minimizing a cost function with **an optimal fit** to the background and observations.

Distance to background **Distance to observations**

$$J(\delta x) = \frac{1}{2}\left(\delta x - \delta x_g\right)^T B^{-1}\left(\delta x - \delta x_g\right) + \frac{1}{2}(H\delta x - d)^T R^{-1}(H\delta x - d)$$

The weighting between the two components is determined by B (background error) and R (observation error).

- A larger B means background is less accurate -> x will get closer to observation
- A larger R means observation is less accurate -> x will get closer to background

Two types of background error covariance (B)

$$J(\delta x) = \frac{1}{2}\left(\delta x - \delta x_g\right)^T B^{-1}\left(\delta x - \delta x_g\right) + \frac{1}{2}(H\delta x - d)^T R^{-1}(H\delta x - d)$$

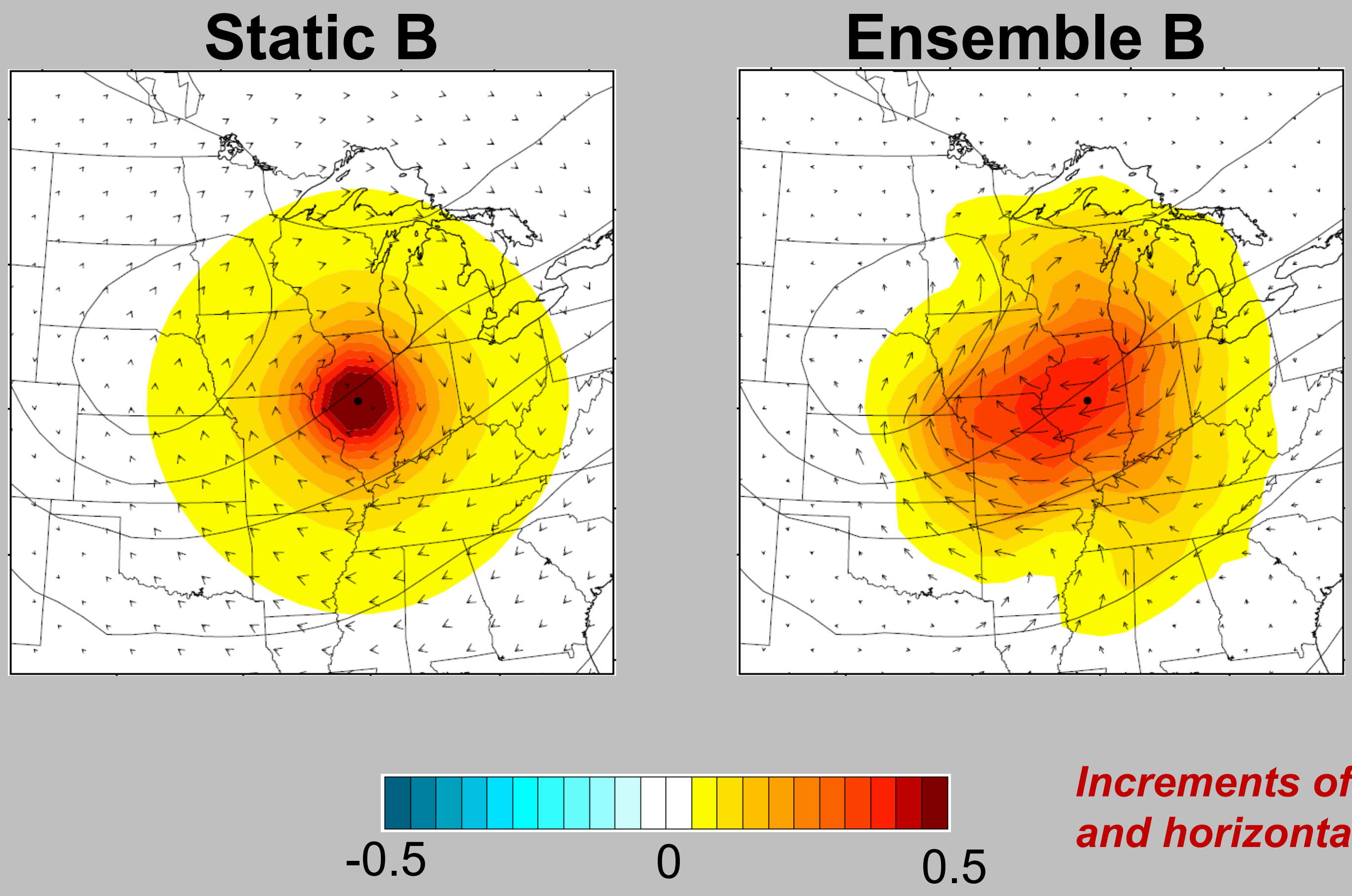
1. **Static B**

   -> from statistic, does not vary with time

2. **Ensemble B**

   -> flow-dependent, reflect the background error in different time

Example to show the B effect (Single observation tests)



Increments of temperature (shaded) and horizontal winds (vector)

Ensemble ***B***:

- Errors of the day are sampled
- flow-dependent update

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Derive B matrix from an ensemble of forecasts

ensemble size

State variable of ensemble mean

$$\boldsymbol{B_e} = \frac{1}{n-1}\sum_{i=1}^{\boldsymbol{n}}(\boldsymbol{x_i} - \boldsymbol{\overline{x}})(x_i - \bar{x})^T$$

State variable of each ensemble member

$$\boldsymbol{B_e} = \frac{1}{n-1}\sum_{i=1}^{\boldsymbol{n}}(\delta x_{\boldsymbol{i}})(\delta x_{\boldsymbol{i}})^T$$

ensemble perturbation

- The ensemble mean provides an estimation of the truth
- The perturbations from the mean estimate the uncertainty, which is used to model background-error covariance matrix.

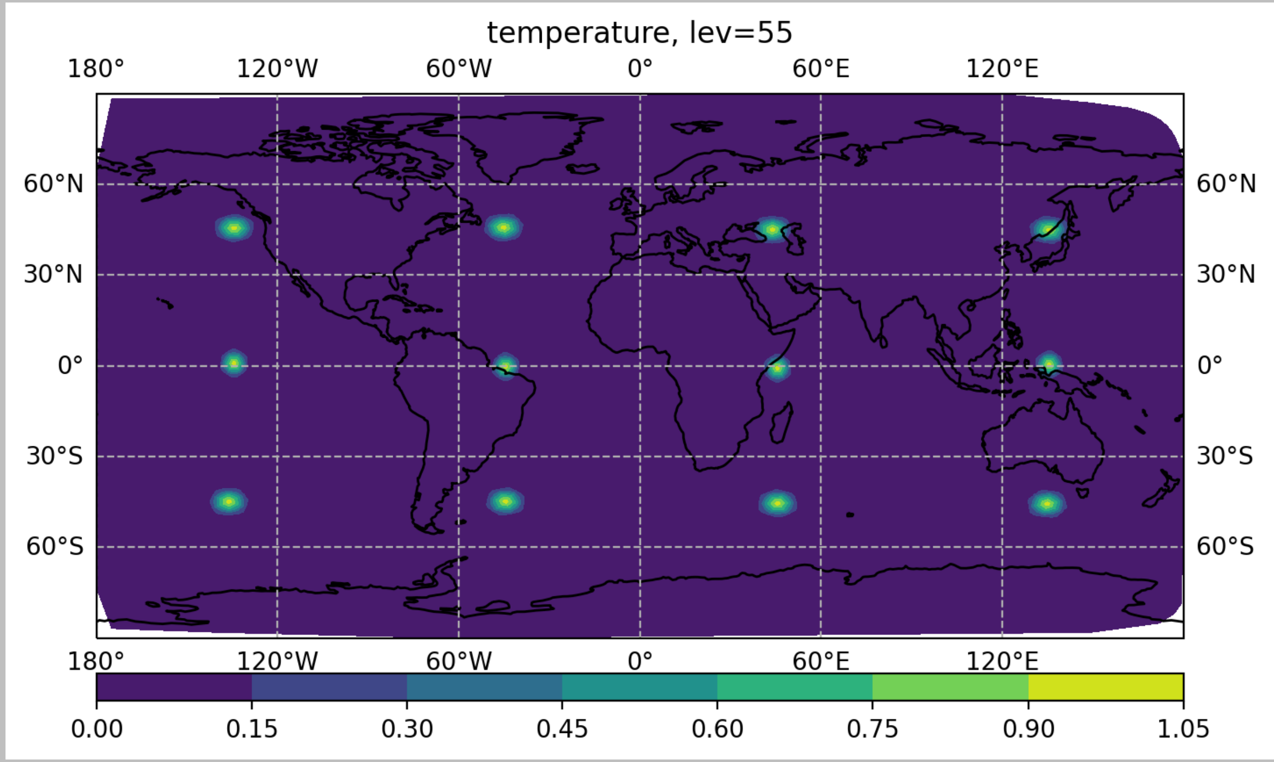
Localization of the *B* matix

Because we do not have a complete estimate of ***B*** (e.g., limited ensemble size) we need to use localization

Basic idea: observations should only influence an area nearby the observation

$$\boldsymbol{B} = \boldsymbol{L} \circ \boldsymbol{B_e}$$

Small localization



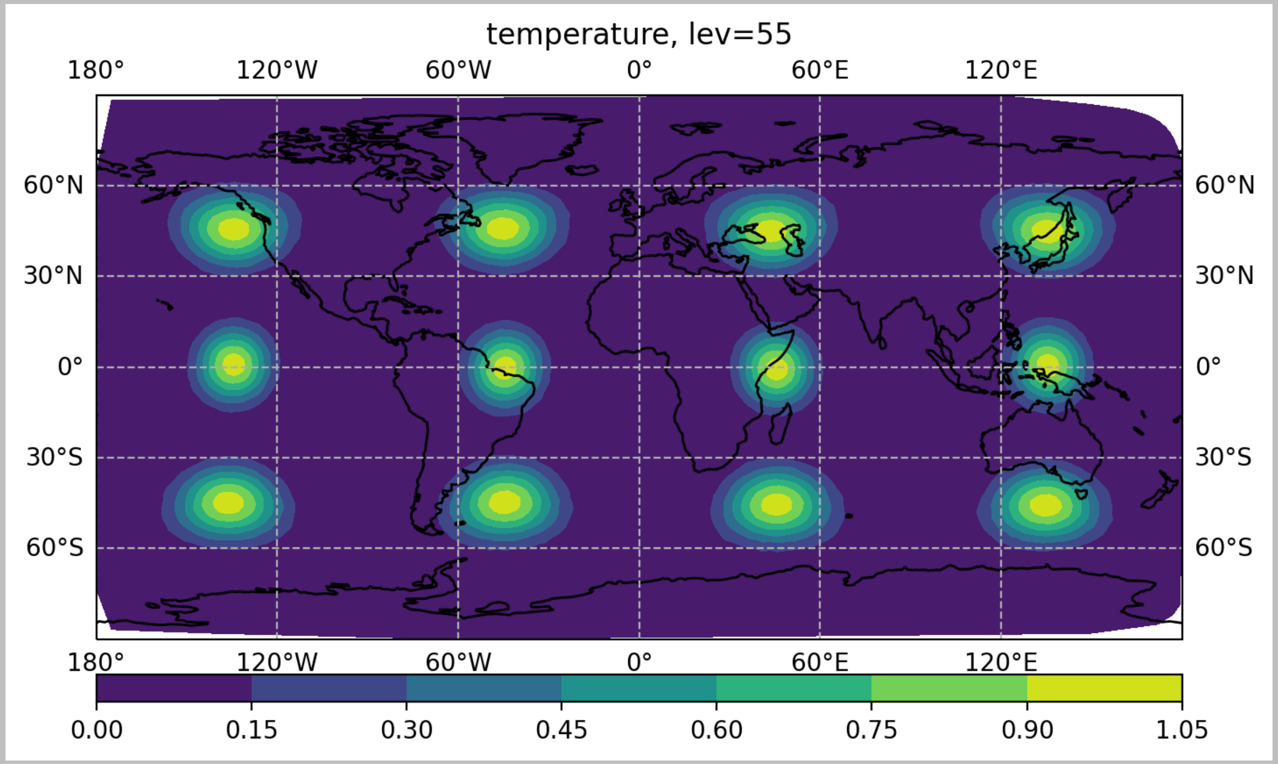
Localization of the *B* matix

Because we do not have a complete estimate of ***B*** (e.g., limited ensemble size) we need to use localization

Basic idea: observations should only influence an area nearby the observation

$$\boldsymbol{B} = \boldsymbol{L} \circ \boldsymbol{B}_e$$

large localization



Benefits of using an ensemble to estimate *B*

- Simple to implement

- Provides a flow-dependent estimate of the errors and uncertainties
  - Depends on the quality of the ensemble

- Incorporates ensemble estimate of background errors within the variational update
  - **Still updates a deterministic forecast**

EnVar uses a pure ensemble B to updates a deterministic forecast

In hybrid methods, B can be a weighting sum between static B ($\boldsymbol{B_s}$) and ensemble B ($\boldsymbol{B_e}$).

$$\boldsymbol{B} = \beta_s \boldsymbol{B_s} + \beta_e \boldsymbol{B_e}$$
$$\beta_s + \beta_e = 1$$

=1

pure ensemble B

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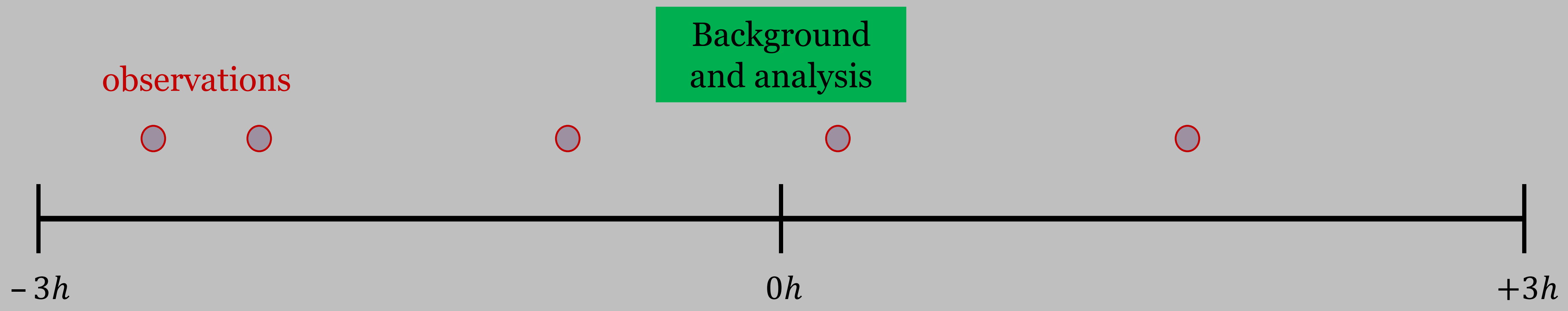
3DEnVar

$$J(x) = \frac{1}{2}(x - x_b)^T \boldsymbol{B}^{-1}(x - x_b) + \frac{1}{2}(h(x) - y)^T \boldsymbol{R}^{-1}(h(x) - y)$$

- We assume that all observations $\boldsymbol{y_o}$ are valid at the same time.
- Usually valid at the center of the window (i.e. at the same time as $\boldsymbol{x}$ and $\boldsymbol{x_b}$)

3DEnVar using a 6h assimilation window



- All observations in 3DEnVar are assumed to be valid at the same time as the background

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Configure the analysis time for 3DEnvar

```
_member config: &memberConfig
  date: &analysisdate '2018-04-15T00:00:00Z'
  state variables: &incvars
  - temperature
  - spechum
  - uReconstructZonal
  - uReconstructMeridional
  - surface_pressure
  stream name: ensemble
cost function:
  cost type: 3D-Var
  window begin: '2018-04-14T21:00:00Z'
  window length: PT6H
  geometry:
    nml_file: "./Data/480km/namelist.atmosphere_2018041500"
    streams_file: "./Data/480km/streams.atmosphere"
    deallocate non-da fields: true
  analysis variables: *incvars
  background:
    state variables: [temperature, spechum, uReconstructZonal, uReconstructMeridional, surface_pressure,
                      theta, rho, u, qv, pressure, landmask, xice, snowc, skintemp, ivgtyp, isltyp,
                      snowh, vegfra, u10, v10, lai, smois, tslb, pressure_p]
    filename: "./Data/480km/bg/restart.2018-04-15_00.00.00.nc"
    date: *analysisdate
```

analysis time (center of window)

Start of assimilation window
length of assimilation window

First guess (should be at analysis time)

Configure the ensemble B

```yaml
background error:
  covariance model: ensemble
  localization:
    localization method: SABER
    saber central block:
      saber block name: BUMP_NICAS
      active variables: *incvars
      read:
        io:
          files prefix: Data/bump/mpas_parametersbump_loc
        drivers:
          multivariate strategy: duplicated
          read local nicas: true
  members:
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig
```

set ensemble *B* for 3DEnVar

Specifying members used to compute ensemble B

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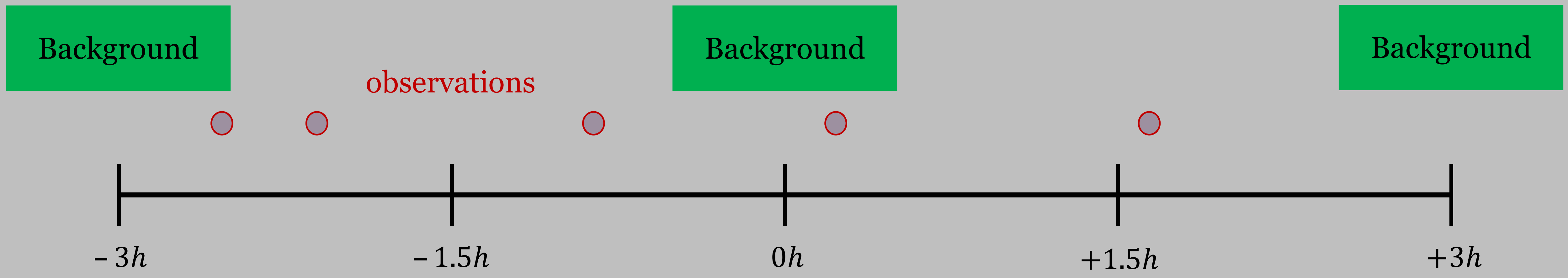
4DEnVar

$$J(x) = \frac{1}{2}(x - x_b)^T B^{-1}(x - x_b) + \frac{1}{2}\sum_{k=1}^{K}(Hx_k - y_k)^T {R_k}^{-1}(Hx_k - y_k)$$

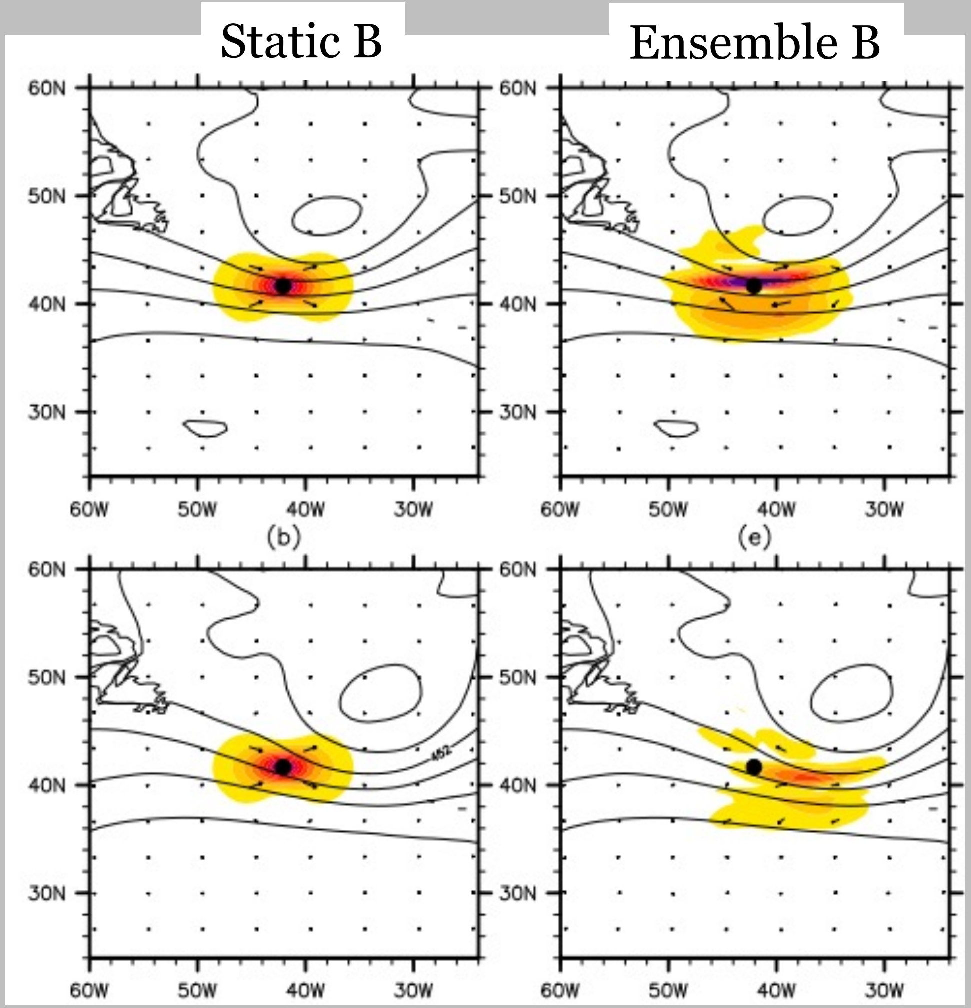


- All observations in 4DEnVar are binned within a smaller subwindow and innovations $(Hx - y_o)$ are calculated relative to background valid at that time.
- Ensemble needed at the center of each subwindow (***K*** ensemble required).

The 4D ensemble *B* is used to propagate the innovation

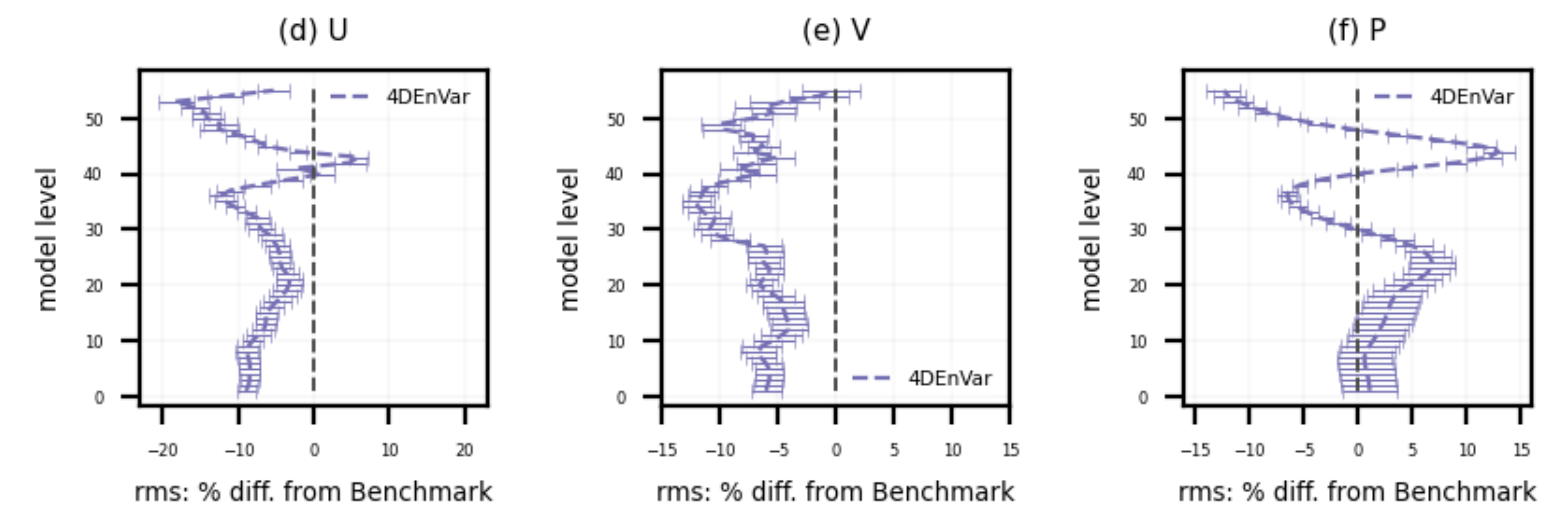
Start of window

end of window



Lorenc et al. (2015)

4DEnVar vs 3DEnVar Performance



- Assimilating observations at their appropriate time improves the analyses

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6. **Setting up a .yaml file for 4DEnVar**

Configure the analysis times for 4DEnvar

```yaml
_member config 1: &memberConfig1
  date: &date1 '2018-04-14T21:00:00Z'
  state variables: &incvars
  - temperature
  - spechum
  - uReconstructZonal
  - uReconstructMeridional
  - surface_pressure
  stream name: ensemble
_member config 2: &memberConfig2
  <<: *memberConfig1
  date: &date2 '2018-04-15T00:00:00Z'
_member config 3: &memberConfig3
  <<: *memberConfig1
  date: &date3 '2018-04-15T03:00:00Z'
cost function:
  cost type: 4D-Ens-Var
  window begin: '2018-04-14T21:00:00Z'
  window length: PT6H
  subwindow: PT3H
```

subwindow1

subwindow2

subwindow3

Background needed for each subwindow

```
cost function:
  cost type: 4D-Ens-Var
  window begin: '2018-04-14T21:00:00Z'
  window length: PT6H
  subwindow: PT3H
  geometry:
    nml_file: "./Data/480km/namelist.atmosphere_2018041500"
    streams_file: "./Data/480km/streams.atmosphere"
  analysis variables: *incvars
  background:
    states:
    - state variables: &stvars
                       [temperature, spechum, uReconstructZonal, uReconstructMeridional, surface_pressure,
                       theta, rho, u, qv, pressure, landmask, xice, snowc, skintemp, ivgtyp, isltyp,
                       snowh, vegfra, u10, v10, lai, smois, tslb, pressure_p]
      filename: "./Data/480km/bg/restart.2018-04-14_21.00.00.nc"
      date: *date1
    - state variables: *stvars
      filename: "./Data/480km/bg/restart.2018-04-15_00.00.00.nc"
      date: *date2
    - state variables: *stvars
      filename: "./Data/480km/bg/restart.2018-04-15_03.00.00.nc"
      date: *date3
```

bg (subwindow 1)

bg (subwindow 2)

bg (subwindow 3)

Configure the ensemble B

```
background error:
  covariance model: ensemble
  localization:
    localization method: SABER
    saber central block:
      saber block name: BUMP_NICAS
      active variables: *incvars
      read:
        io:
          files prefix: Data/bump/mpas_parametersbump_loc
        drivers:
          multivariate strategy: duplicated
          read local nicas: true
```

set ensemble *B* for 4DEnVar

Member file needed for each subwindow

```yaml
members:
- states:
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem01/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem02/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem03/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem04/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
- states:
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-14_21.00.00.nc
    <<: *memberConfig1
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-15_00.00.00.nc
    <<: *memberConfig2
  - filename: Data/480km/bg/ensemble/mem05/x1.2562.init.2018-04-15_03.00.00.nc
    <<: *memberConfig3
```

Further reading: an alternative way to specify the *B* ensemble

```yaml
- covariance:
    covariance model: ensemble
    localization:
      localization method: SABER
      saber central block:
        saber block name: BUMP_NICAS
        active variables: *incvars
        read:
          io:
            files prefix: Data/bump/mpas_parametersbump_loc
          drivers:
            multivariate strategy: duplicated
            read local nicas: true
    members from template:
      template:
        <<: *memberConfig
        filename: Data/480km/bg/ensemble/mem%iMember%/x1.2562.init.2018-04-15_00.00.00.nc
      pattern: '%iMember%'
      start: 1
      zero padding: 2
      nmembers: 4
      except: [1] # chooses 2, 3, 4, 5
```

You can find it at
./mpas_bundle_v2/build/mpas-jedi/test/testinput /eda_3dhybrid_1.yaml

References

- Liu, Z., and Coauthors, 2022: Data assimilation for the Model for Prediction Across Scales - Atmosphere with the Joint Effort for Data assimilation Integration (JEDI-MPAS 1.0.0): EnVar implementation and evaluation. *Geosci. Model Dev.*, **15**, 7859–7878, https://doi.org/10.5194/gmd-15-7859-2022.
- Lorenc, A. C., N. E. Bowler, A. M. Clayton, S. R. Pring, and D. Fairbairn, 2015: Comparison of hybrid-4DEnVar and hybrid-4DVar data assimilation methods for global NWP. *Mon. Weather Rev.*, **143**, 212–229, https://doi.org/10.1175/MWR-D-14-00195.1.